Why matrix norm is important?

You know that a computer cannot represent real numbers exactly unless they are dyadic numbers.

$1.d_1 d_2 \cdots d_t \times 2^e$

So, suppose you want to solve

$$A\mathbf{x} = \mathbf{b}, \quad A \in \mathbb{R}^{m \times m}$$

But in reality, you have to encode A, $\mathbf{x}$, $\mathbf{b}$ on the computer.
Let $A' = fl(A)$, $\mathbf{x}' = fl(\mathbf{x})$, $\mathbf{b}' = fl(\mathbf{b})$.
i.e., you end up solving

$$A'\mathbf{x}' = \mathbf{b}'$$

Suppose for the moment, let's assume $\mathbf{b}' = \mathbf{b}$ for simplicity.
Now, you want to know the relative error of the solution:

$$\frac{\|\mathbf{x}' - \mathbf{x}\|}{\|\mathbf{x}'\|} = \frac{\|\mathbf{x}' - A^{-1}\mathbf{b}\|}{\|\mathbf{x}'\|}$$

rel. error in solution

$$= \frac{\|\mathbf{x}' - A^{-1}A'\mathbf{x}'\|}{\|\mathbf{x}'\|}$$

$$= \frac{\|A^{-1}(A - A')\mathbf{x}'\|}{\|\mathbf{x}'\|}$$

$$\leq \frac{\|A^{-1}\| \cdot \|A - A'\| \cdot \cancel{\|\mathbf{x}'\|}}{\cancel{\|\mathbf{x}'\|}}$$

$$= \underbrace{\|A\|\,\|A^{-1}\|}_{\text{amplification factor}} \; \underbrace{\frac{\|A - A'\|}{\|A\|}}_{\text{relative error in matrix}}$$

Now define the condition number of A by

$$\kappa(A) = \mathrm{cond}(A) := \|A\| \cdot \|A^{-1}\|$$

If $\kappa(A)$ is large, then A is pretty bad, i.e., $\exists$ large error in solution $\mathbb{x} = A^{-1}\mathbb{b}$.

- Roughly speaking, to compute A^{-1} or the solution of $A\mathbb{x} = \mathbb{b}$, we lose $\approx \log_{10} \kappa(A)$ digits.
- In particular, if A is singular, $\kappa(A) = +\infty$.

A Brief Intro to Least Squares Problem

Since the error analysis of Gaussian elimination & LU decomposition are subtle and difficult, we'll first talk about the least squres problem, then talk about the projections, QR decomposition, etc.

The Least Squares Problem was conceived by Gauss and Legendre around 1800 in the fields of astronomy & geodesy, in particular, model fitting to measured data.

Want to solve

$$(*) \quad A\mathbf{x} = \mathbf{b}$$

overdetermined

where $A \in \mathbb{R}^{m\times n}$, $m > n$, $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{b} \in \mathbb{R}^m$

more equations than unknowns

In general, (*) has no exact solution unless $\mathbf{b} \in \text{range}(A)$.

this usually does not happen!

$\Rightarrow$ Check the size of the residual

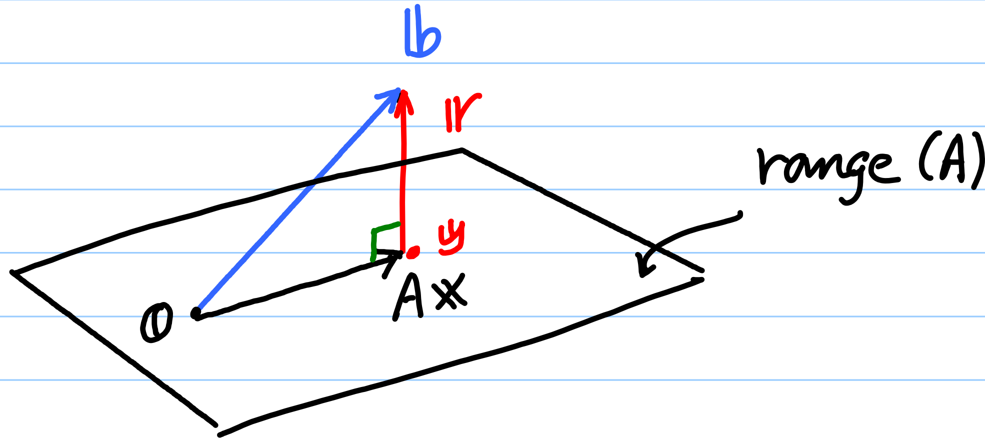
$$\mathbf{r} := \mathbf{b} - A\mathbf{x} \in \mathbb{R}^m$$

and want $\mathbf{r}$ as small as possible.

$$\begin{cases} \text{Given } A \in \mathbb{R}^{m\times n},\ m \ge n,\ \mathbf{b} \in \mathbb{R}^m \\ \text{Find } \mathbf{x} \in \mathbb{R}^n \text{ s.t. } \|\mathbf{b} - A\mathbf{x}\|_2 \to \min \end{cases}$$

This is called a general linear least squares problem.

why 2-norm is used?
$\Rightarrow$ its geometric interpretation!



Thm. Let $A \in \mathbb{R}^{m \times n}$, $m \geq n$, $b \in \mathbb{R}^m$.
Then, $x \in \mathbb{R}^n$ is the minimizer of

$$\| r \|_2 = \| b - Ax \|_2$$

$\Longleftrightarrow \quad r \perp \text{range}(A)$

$\Longleftrightarrow \quad A^T r = 0$

$\Longleftrightarrow \quad A^T A x = A^T b$ (The normal equation)

$\Longleftrightarrow \quad A(A^T A)^{-1} A^T b = Ax$

Furthermore,
$A^T A$ is nonsingular $\Longleftrightarrow$ A is full rank
Consequently, rank(A) = n if $m \geq n$
The solution x is unique $\Longleftrightarrow$ A: full rank

(Proof) These statements are essentially obvious from the figure.

also $\mathbf{r} \perp \text{range}(A)$

$$\iff \mathbf{r} \perp \mathbf{a}_j \quad 1 \le j \le n$$

$$\iff \mathbf{r}^T [\mathbf{a}_1 \cdots \mathbf{a}_n] = \mathbf{0}$$

$$\iff \mathbf{r}^T A = \mathbf{0} \iff A^T \mathbf{r} = \mathbf{0}$$

Then
$$\begin{aligned} A^T \mathbf{r} &= A^T(\mathbf{b} - A\mathbf{x}) \\ &= A^T\mathbf{b} - A^TA\mathbf{x} \\ &= \mathbf{0} \end{aligned}$$

$$\iff A^TA\mathbf{x} = A^T\mathbf{b} \quad \checkmark$$

Now we can also show the uniqueness of the orthogonal projection of $\mathbf{b}$ onto range(A) as follows:

Let $\mathbf{y} = A\underline{(A^TA)^{-1}A^T\mathbf{b}} \in \text{range}(A)$

which obviously minimize $\underbrace{\|\mathbf{b} - \mathbf{y}\|_2}_{= \mathbf{r}}$

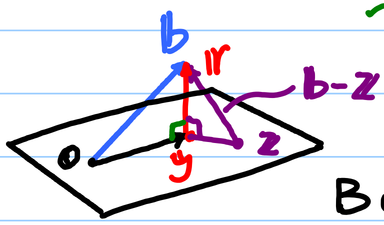
Suppose $\exists\, \mathbf{z} \neq \mathbf{y}$ s.t.

$$\|\mathbf{b} - \mathbf{z}\|_2 = \|\mathbf{b} - \mathbf{y}\|_2, \quad \mathbf{z} \in \text{range}(A)$$

Then, $\mathbf{y} - \mathbf{z} \in \text{range}(A)$.

So, $\mathbf{y} - \mathbf{z} \perp \mathbf{b} - \mathbf{y}$

$$\iff \|\mathbf{b} - \mathbf{z}\|_2^2 \underset{\uparrow}{=} \|\mathbf{b} - \mathbf{y}\|_2^2 + \|\mathbf{y} - \mathbf{z}\|_2^2$$



Pythagoras!

But these two are equal by the assumption.

so $\|\mathbf{y} - \mathbf{z}\|_2 = 0 \iff \mathbf{y} = \mathbf{z}$ #

- $(A^T A)^{-1} A^T$ is often called pseudoinverse of A, and denoted by $\underline{\underline{A^+}}$

- What happens if $m < n$? This case is called underdetermined. $\underset{\text{many sol's.}}{\text{infinitely}}$

Need extra constraints to solve such LS problem, e.g., $\min \|\mathbf{x}\|_2$

That is,

Find $\mathbf{x} \in \mathbb{R}^n$, s.t.

$$\min \|\mathbf{x}\|_2^2 \text{ subject to } A\mathbf{x} = \mathbf{b}.$$

This is done by the Lagrange multipliers:

Let $J(\mathbf{x}) := \mathbf{x}^T \mathbf{x} + \lambda^T(\mathbf{b} - A\mathbf{x})$

$\lambda \in \mathbb{R}^m$

Then want $\min J(\mathbf{x})$.

$$\frac{\partial J}{\partial \mathbf{x}} = 2\mathbf{x} - A^T \lambda = \mathbf{0}$$

$\iff \hat{\mathbf{x}} = \frac{1}{2} A^T \lambda$, this $\hat{\mathbf{x}}$ minimizes $J(\mathbf{x})$

Now, $\mathbf{b} = A\mathbf{x} = \frac{1}{2} A A^T \lambda$

$\iff \lambda = 2(AA^T)^{-1}\mathbf{b}$

$\iff \hat{\mathbf{x}} = \frac{1}{2} A^T \lambda = \underline{A^T (AA^T)^{-1} \mathbf{b}}$

compare this with $(A^T A)^{-1} A^T \mathbf{b}$ in the case of $m \geq n$.

Example The LS polynomial fit

Given m distinct points $x_1, \cdots, x_m \in \mathbb{R}$
and data $y_1, \cdots, y_m \in \mathbb{R}$
Want to fit a polynomial of deg. $n-1$

$$p(x) = c_0 + c_1 x + \cdots + c_{n-1} x^{n-1}$$

for some $n < m$.
Such a polynomial is a LS fit to the data if it minimizes the residual

$$(*) \quad \sum_{i=1}^{m} |p(x_i) - y_i|^2.$$

So,

$$\underbrace{\begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ \vdots & & & & \vdots \\ 1 & x_m & x_m^2 & \cdots & x_m^{n-1} \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} c_0 \\ \vdots \\ c_{n-1} \end{bmatrix}}_{\mathbf{x}} \approx \underbrace{\begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}}_{\mathbf{b}}$$

vandermonde! $\quad (*) = \|\mathbf{r}\|_2^2 = \|\mathbf{b} - A\mathbf{x}\|_2^2$

MATLAB Demo here!